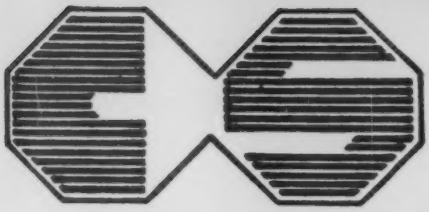

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(*b*) **electronic** (visible, absorption and emission)

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(*c*) **photoelectron**

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(*d*) electron spin resonance

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(*e*) nuclear magnetic resonance, quadrupole resonance

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(*f*) neutron scattering

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(*g*) ion cyclotron resonance, mass spectrometry *etc.*

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THE FIFTH ANNUAL GENERAL MEETING OF THE FARADAY DIVISION of The Chemical Society was held at 9.00 a.m., on 9th September 1976, in the Molecular Sciences Lecture Theatre, The University of Sussex, with Professor D. H. Everett, M.B.E., M.A., D.Sc., C.Chem., F.R.I.C., in the Chair.

1 *Minutes*

The Minutes of the Fourth Annual General Meeting of the Faraday Division, which had been circulated previously, were taken as read and confirmed.

2 *Annual Report*

During 1975 the Faraday Division held two General Discussions and one Symposium. The first Discussion, No. 59 on 'Physical Adsorption in Condensed Phases' was held at the University of Bristol in April and attracted more than 150 participants including 35 from overseas. The second Discussion, No. 60, on 'Electron Spectroscopy of Solids and Surfaces' was held at the University of British Columbia, Vancouver, Canada in July and was the 5th Faraday Discussion to be held in North America since 1952. About 170 participants attended the Discussion including 35 from outside North America and 55 from the U.S.A. The Division was indebted to Professor McDowell for the initial invitation to visit Canda, and to him and his Canadian Organisation for their most successful efforts in obtaining financial support from the University of British Columbia, The Chemical Institute of Canada, Physical Chemistry Division, North American industry (*viz.* Atomic Energy of Canada, Canadian Marconi Company, Dow Chemical Company, Dupont of Canada, Fisher Scientific Company, Imperial Oil Ltd., National Research Council, Research Corporation of America), and the Government of British Columbia. The Faraday also recorded its grateful thanks to the Royal Society for a generous contribution towards the travel expenses of the European participants. Symposium No. 10 on 'Proton Transfer' was held at Stirling in September and coincided with the retirement of Professor R. P. Bell who opened the meeting with the 17th Spiers Memorial Lecture entitled 'The Development of Ideas about Proton Transfer Reactions'. 150 participants were present at the Symposium including over 50 from overseas.

In addition to the published meetings the Division was also represented at the Annual Congress at York, in April, where a Symposium was arranged jointly with Perkin Division and E.S.R. Group on 'Electron Spin Resonance Spectroscopy of Free Radicals' and at the Autumn Meeting in Reading where an informal discussion on 'Interpretations of the Properties of Naturally Occurring Multicomponent Solutions such as Sea Water and Body Fluid' was held. An informal half day meeting was arranged in London on 'Photogalvanic and Photovoltaic Aspects of Solar Energy Conversion' and the Division collaborated with the Institute of Physics on a meeting on 'Interatomic Forces in Condensed Matter' held at Reading in April.

The 1975 Bourke Lectures entitled 'Kinetic Information from Chemical Lasers' were given by Professor G. C. Pimentel (University of California, Berkeley, U.S.A.) at the Universities of Cardiff, Reading and Heriot-Watt. The Centenary Lecture by Professor R. Hoffmann (Cornell University, U.S.A.) on 'Theoretical Aspects of Penta-Coordination' was allocated to the Faraday and Dalton Division and was given at a half-day Symposium in London.

The Marlow Medal for 1975 was awarded to Dr. G. Duxbury (University of Bristol) for his contributions to many aspects of experimental and theoretical spectroscopy.

It was with great regret that Council recorded in November, the death of Professor J. W. Linnett, F.R.S. Professor Linnett was the last President of the Faraday Society and the first President of the Faraday Division. At the time of his death he was a Vice-President of the Division and the President Elect of The Chemical Society.

In 1975 the eight subject groups affiliated to the Division continued to make valuable contributions by arranging specialist group meetings which included meetings on the following topics:

Applications of Lasers in Chemical Kinetics (Gas Kinetics Group)
Phase Separation and Phase Equilibrium in Polymer Solutions (Polymer Physics Group)
The Hydrogen Economy (Electrochemistry Group)

Potential Energy Surfaces (Theoretical Chemistry Group)
Surface Science (Surface Reactivity and Catalysis Group)
Rheometry (Polymer Physics Group)
Molecular Spectroscopy and Neutron Scattering (Neutron Scattering Group)
Electrochemistry of Lead (Electrochemistry Group)
Excitations of Surfaces and Adsorbed Molecules (Neutron Scattering Group)
International Symposium on Gas Kinetics (Gas Kinetics Group)
Molecular Beams (Molecular Beam Kinetics Group)
Polymers at the Liquid–Solid Interface (Colloid and Interface Science Group)
Chemisorption and Catalysis (Surface Reactivity and Catalysis Group)
Organic Electrochemical Synthesis (Electrochemistry Group)
Novel Electrode Materials (Electrochemistry Group)
Pseudo Potentials (Theoretical Chemistry Group)
Electrical Methods of Machining, Forming and Coating (Electrochemistry Group)
Diffuse and Small-angle Neutron Scattering from Disordered Materials (Neutron Scattering Group)
Spin Waves (Neutron Scattering Group)
Mass Transport in Ceramic Materials (Electrochemistry Group)
The Structure and Dynamics of Liquids (Neutron Scattering Group)

Membership of the Division in 1975 was 4,363 comprising 2,903 U.K. members and 1,460 members from overseas.

Faraday Division Newsletter No. 2 was distributed to members with the February issue of 'Chemistry in Britain'.

3 *Treasurer's Report*

The Treasurer reported on the action taken by Council following the resolution passed in 1975 'that Council be requested to seek an increase in the allocation of funds to the Faraday Division for the organising of conferences'. At the time of the resolution, it had not been possible to increase the funds because all Divisions had agreed to freeze expenditure at the 1974 level for a period of 3 years. However, that period was over in 1976/7 and a request by all Divisions for a 50% increase in the allocation to the Divisions Committee had been granted and a decision on the allocations to individual Divisions was awaited. In the meantime, it had been possible to increase by 50% the sum available to Organising Committees following a decision that the income from the sale of preprints be accrued to the Faraday Division.
In 1976, it had also been agreed that a Division making a saving against its 'other cost' budget would be allowed to carry forward to the following year, half the saving achieved up to a maximum of half the annual allocation to the Division.

4 *Elections to Council*

The members of the Council of the Faraday Division of The Chemical Society to take office from March 1977 were as follows:

President

PROF. D. H. EVERETT, M.B.E., M.A., D.Sc., C.Chem., F.R.I.C.

Vice-Presidents who have held office as President

PROF. C. E. H. BAWN, C.B.E., Ph.D., F.R.S.
PROF. G. GEE, C.B.E., Sc.D., C.Chem., F.R.I.C., F.R.S.
PROF. SIR GEORGE PORTER, M.A., Sc.D., C.Chem., F.R.I.C., F.R.S.
DR. T. M. SUGDEN, C.B.E., M.A., Sc.D., C.Chem., F.R.I.C., F.R.S.
PROF. R. P. BELL, M.A., C.CHEM., F.R.I.C., F.R.S., F.R.S.E.

Vice-Presidents

PROF. A. D. BUCKINGHAM, M.A., Ph.D., C.Chem., F.R.I.C., F.R.A.C.I., F.R.S.
PROF. P. GRAY, M.A., Sc.D., C.Chem., F.R.I.C.
PROF. M. MAGAT, D.Sc., D.Phil.
PROF. J. S. ROWLINSON, M.A., D.Phil., C.Chem., F.R.I.C., F.R.S.
DR. H. A. SKINNER, B.A., D.Phil., C.Chem., F.R.I.C.
PROF. F. C. TOMPKINS, D.Sc., C.Chem., F.R.I.C., F.R.S.
PROF. D. H. WHIFFEN, M.A., D.Phil., D.Sc., C.Chem., F.R.I.C., F.R.S.

Ordinary Members

Dr. W. J. Albery, M.A. D. Phil.
Dr. J. H. Baxendale, D. Sc.
Prof. Mansel Davies, Sc.D., C.Chem., F.R.I.C.
Dr. W. J. Dunning, M.B.E., Ph.D., C.Chem., F.R.I.C.
Prof. F. Franks, D.Sc., C.Chem., F.R.I.C.
Dr. D. N. Hague, M.A., Ph.D., C.Chem., F.R.I.C.
Dr. G. R. Luckhurst, Ph.D.
Prof. A. M. North, D.Sc., F.R.S.E., C.Chem., F.R.I.C.
Dr. B. A. Thrush, M.A., Sc.D.
Dr. D. A. Young, D.Sc., M.Inst.P.

Honorary Secretary

Prof. F. C. Tompkins, D.Sc., C.Chem., F.R.I.C., F.R.S.

Honorary Treasurer

Prof. P. Gray, M.A., Sc.D., C.Chem., F.R.I.C.

The President thanked Professor W. C. Price, Professor N. B. H. Jonathan, Professor I. M. Mills, Dr. R. Parsons and Dr. B. A. Pethica, the retiring members of Council, for their services.

5 *Future Activities*

The President reviewed future activities of the Faraday Division and drew attention to the increase in Divisional activities since amalgamation. A full programme of Discussions and Symposia was planned for 1977 and the Division would also contribute informal discussions to the Annual and Autumn Meetings of the Society. In addition to the Bourke Lectures by Professor R. Gordon (Harvard), the Division would also be allocated half-day Symposia arranged around endowed lectures of the Society and the President reminded members that these were Faraday meetings and urged them to encourage colleagues to support them.

Council was continuing to collaborate with other Societies; the second of the biennial Joint Meetings with the Deutsche Bunsen Gesellschaft, the Société de Chimie Physique and the Associazione Italiana di Chimica Fisica was to be held in Germany in 1976 and the third was planned for France in 1978. Also, two meetings sponsored jointly with the Institute of Physics were to take place in September 1977.

Professor Murrell proposed that members of the Division be reminded that they were invited to suggest topics for Discussions and it was agreed that a notice to this effect should appear in the Faraday Transactions and in 'Chemistry in Britain'.

NOTICES TO AUTHORS—No. 7/1970

Deposition of Data—Supplementary Publications Scheme

Preamble

The growing volume of research that produces large quantities of data, the increasing facilities for analysing such data mechanically, and the rising cost of printing are each making it very difficult to publish in the *Journal* in the normal way the full details of the experimental data which become available. Moreover, whilst there is a large audience for the general method and conclusions of a research project, the number of scientists interested in the details, and in particular in the data, of any particular case may be quite small. The British Library Lending Division (B.L.L.D.) in consultation with the Editors of scientific journals, has now developed a scheme whereby such data and detail may be stored and then copies made available on request at the B.L.L.D., Boston Spa. The Chemical Society is a sponsor of this scheme and has indicated to the B.L.L.D. its wish to use the facilities being made available in this "Supplementary Publications Scheme".

Bulk information (such as crystallographic structure factor tables, computer programmes and output, evidence for amino-acid sequences, spectra, *etc.*), which accompany papers published in future issues of the Chemical Society's *Journal* may in future be deposited, free of charge, with the Supplementary Publications Scheme, either at the request of the author and with the approval of the referees or on the recommendation of referees and the approval of the author.

The Scheme

Under this scheme, authors will submit articles and the supplementary material to the *Journal* simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication the supplementary material will be sent by the Society to the B.L.L.D. where it will be stored. Copies will be obtainable by individuals both in the U.K. and abroad on quoting a supplementary publication number that will appear in the parent article.

Preparation of Material

Authors will be responsible for the preparation of camera-ready copy according to the following specifications (although the Society will be prepared to help in case of difficulty).

(*a*) Optimum page size for text or tables in typescript: up to 30 cm × 21 cm.

(*b*) Limiting page size for text or tables in typescript: 33 cm × 24 cm.

(*c*) Limiting size for diagrams, graphs, spectra, *etc.*: 39 cm × 28·5 cm.

(*d*) Tabular matter should be headed descriptively on the first page, with column headings recurring on each page.

(*e*) Pages should be clearly numbered.

It is recommended that all material which is to be deposited should be accompanied by some prefatory text. Normally this will be the summary from the parent paper and authors will greatly aid the deposition of the material if a duplicate copy of the summary is provided. If authors have the facilities available the use of a type face designed to be read by computers is encouraged.

Deposition

The Society will be responsible for the deposition of the material with the B.L.L.D. The B.L.L.D. will not receive material direct from authors since the Library wishes to ensure that the material has been properly and adequately refereed.

Action by the Society

The Society will receive a manuscript for publication together with any supplementary material for deposition and will circulate all of this to referees in the normal way. When the edited manuscript is sent to the printers the supplementary material will be sent for deposition to the National Lending Library who will issue the necessary publication number. The Society will add to the paper, at the galley proof stage, a footnote indicating what material has been deposited in the Supplementary Publications Scheme, the number of pages it occupies, the supplementary publication number, and details as to how copies may be obtained.

Availability

Copies of Supplementary Publications may be obtained from the B.L.L.D. on demand by organisations which are registered borrowers. They should use the normal forms and coupons they use for all requests. Others may obtain them at the rates shown below. Costs include postage (airmail where available). Cheques should be made payable to 'The British Library'. Hard copy will normally be provided.

United Kingdom	5p per page
Europe	£1.25 per 10 pages
Outside Europe	£1.65 per 10 pages.

Pro forma invoices are sent in all cases where normal forms and coupons are not used. All requests for Supplementary Publications should be addressed as follows:

M. J. P. Chillag,
British Library Lending Division,
Boston Spa,
Wetherby,
West Yorkshire LS23 7BQ,
United Kingdom.

In all correspondence with the B.L.L.D. or the Society authors must cite the supplementary publication number.

International Collaboration

A similar scheme (known as the National Auxiliary Publications Service) is being operated in the U.S.A. by the American Society for Information Science. Similar schemes are also being contemplated in other countries. The provision of reciprocal arrangements for the exchange of supplementary data between the various national deposition centres is being investigated.

NOTICE TO AUTHORS—No. 9/1974

Nomenclature

For many years the Society has actively encouraged the use of standard I.U.P.A.C. nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. Although the I.U.P.A.C. rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general.

In order to encourage authors to use I.U.P.A.C. nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given.

'Nomenclature of Organic Chemistry, Sections A, B, and C', Butterworths, London, 2nd Edition, 1971.

'Nomenclature of Inorganic Chemistry', Butterworths, London, 1971.

'Manual of Symbols and Terminology for Physicochemical Quantities and Units', Butterworths, London, 1970.

In addition to the above publications, provisional rules for the naming of organometallic compounds, amino-acids, carbohydrates, carotenoids, and steroids, and rules of stereochemistry are available from the:

I.U.P.A.C. Secretariat,
Bank Court Chambers,
2-3 Pound Way,
Cowley Centre,
OXFORD OX4 3YF.

It is recommended that where there are no I.U.P.A.C. rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff.

NOTICE TO AUTHORS—No. 10/1976

Authentication of New Compounds

(1) It is the responsibility of authors to provide fully convincing evidence for the homogeneity and identity of all compounds they claim as new. Evidence of both purity and identity is required to establish that the properties and constants reported are those of the compound with the new structure claimed.

(2) In the context of this Notice a compound is considered as new (*a*) if it has not been prepared before, (*b*) if it has been prepared before but not adequately purified, (*c*) if it has been purified but not adequately characterised, (*d*) if, earlier, it has been assigned an erroneous constitution, or (*e*) if it is a natural product synthesised for the first time. In preliminary communications compounds are often recorded with limited characterising data; in spite of (*c*) above later preparations of such compounds are not considered as new if the properties previously reported are confirmed; the same applies to patents.*

(3) Referees are asked to assess, as a whole, the evidence in support of the homogeneity and structure of all new compounds. No hard and fast rules can be laid down to cover all types of compounds, but the Society's policy remains unchanged in that evidence for the unequivocal identification of new compounds should normally include good elemental analytical data; an accurate mass measurement of a molecular ion does not provide evidence of purity of a compound and must be accompanied by independent evidence of homogeneity. Low-resolution mass spectroscopy must be treated with even more reserve in the absence of firm evidence to distinguish between alternative molecular formulae. Where elemental analytical data are not available, appropriate evidence which is convincing to an expert in the field will be acceptable, but authors should include, for the referees, a brief explanation of the special nature of their problem.

(4) Spectroscopic information necessary to the assignment of structure should normally be given. Just how complete this information should be must depend upon the circumstances; the structure of a compound obtained from an unusual reaction or isolated from a natural source needs much stronger supporting evidence than one derived by a standard reaction from a precursor of undisputed structure. Authors are reminded that full spectroscopic assignments may always be treated as a Supplementary Publication where their importance does not justify their inclusion in the published paper.

(5) Finally, referees are reminded of the need to be exacting in their standards but at the same time flexible in their admission of evidence. It remains the Society's policy to accept work only of high quality and to permit no lowering of present standards.

* New compounds should be indicated by underlining the name (for italics) at its first mention (excluding headings) in the Experimental section only, and by giving analytical results in the form: (Found: C, 63.1; H, 5.4. $C_{13}H_{13}NO_4$ requires C, 63.2; H, 5.3 %). If analytical results for compounds which have been adequately described in the literature are to be included, they should be given in the form: (Found: C, 62.95; H, 5.4. Calc. for $C_{13}H_{13}NO_4$: C, 63.2; H, 5.3 %). Analyses are normally quoted to the nearest 0.05 %.

Publication of Theoretical and Computational Papers

The Primary Journals Committee has been considering future policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programs. Many such papers report what would be considered 'routine work' in other areas of chemistry and have often included extensive detail.

A specialist sub-committee formulated a set of proposals which were circulated to a large representative sample of theoretical chemists and met with general acceptance. These, with the comments on them, form the basis of this notice.

The Primary Journals Committee recognises that computational work can play a valuable role in chemistry, and will probably continue to do so on an increasing scale. It accepts the time-honoured principle that the first criterion for publication of a paper by the Society should be the worthiness of the chemical problem considered, rather than the particular techniques employed by the author. For example, the use of a new computing algorithm, or the modification of a program, would not usually, on its own, provide sufficient justification for publication.

The Primary Journals Committee recommends to authors the following guidelines for the preparation of computational papers, so that the material can be presented concisely and effectively.

(i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to Faraday Transactions II, one in which the computations are incidental to the chemistry to Perkin, Dalton or Faraday I Transactions. Papers concerned mainly with computational details are unlikely to be accepted.

(ii) The purpose of the paper and the precise objectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.

(iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer program used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.

(iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.

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